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FOREWORD INTRODUCTION

3-Buten-2-ol, 2-methyl-

CAS N°: 115-18-4

SIDS Initial Assessment Report

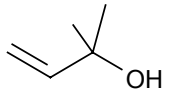
For

SIAM 4

Ispra, Italy, 23 - 25 October 1995

1. Chemical Name:	3-Buten-2-ol, 2-methyl-
2. CAS Number:	115-18-4
3. Sponsor Country:	Switzerland SIDS Contact Point in Sponsor Country: Mr. Georg Karlaganis
4. Shared Partnership with:	
5. Roles/Responsibilities of the Partners:	
• Name of industry sponsor /consortium	
• Process used	
6. Sponsorship History	
• How was the chemical or category brought into the OECD HPV Chemicals Programme ?	SIDS Dossier discussed at the 2nd and 3rd SIDS Review Meetings, March and September 1993. Agreed that the testing plan should be revised to include genotoxicity testing. Results for this test obtained from Germany and circulated to SIDS Contact Points.
7. Review Process Prior to the SIAM:	
8. Quality check process:	
9. Date of Submission:	26 June 1995
10. Date of last Update:	
11. Comments:	At the 3rd Review Meeting it was agreed that the following tests should be done: • 28-day Repeated Dose • Chromosomal Aberration in vivo • Preliminary Reproduction Toxicity Screening Test. After the meeting the sponsor company received a copy of the German study report "Cytogenetic Study in Vivo of 2-Methylbuten-3-ol-2 in Mice; Micronucleus Test". The SIDS Contact Points were then informed of the availability of this test and of the revision of the testing plan saying that only the Repeated Dose and the Reprotox studies would be performed. The Contact Points did not receive a copy of the test results.

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	115-18-4
Chemical Name	2-Methyl-3-butene-2-ol
Structural Formula	

CONCLUSIONS AND RECOMMENDATIONS

It is currently considered of low potential risk and low priority for further work.

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE CONCLUSIONS AND RECOMMENDATIONS

The production volume in Switzerland is about 10,000 tons/year. This chemical is mainly used as starting material or intermediate in the synthesis of drugs, vitamins, flavoring agents etc. Minor amounts are used as attractant in bark beetle traps. The chemical is a natural constituent of hops.

This chemical is of low acute toxicity for water organisms. It is readily biodegradable and no bioaccumulation is expected. The identified uses and the PEC/PNEC considerations derived from the available data do not indicate concern for the environment.

This chemical is of low acute toxicity and is not genotoxic. It is irritating to the eyes but not to the skin. The lowest NOAEL determined was 50mg/kg/day. Based on the available exposure information no concern for consumers and workers could be identified.

NATURE OF FURTHER WORK RECOMMENDED

No further studies are required to evaluate potential health and environmental effects.

FULL SIDS SUMMARY

CAS NO: 115-18-4		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point	NA	not specified	-26 °C
2.2	Boiling Point	NA	DIN 51751	96 - 98.5 °C (at 101.3 kPa)
2.3	Density	NA	DIN 51757	0.82 g/cm³
2.4	Vapour Pressure	NA	calculated measured	3.13 kPa at 25 °C 13.02 kPa at 50°C
2.5	Partition Coefficient (Log Pow)	NA	OECD 107	0.66
2.6 A.	Water Solubility	NA	not specified	190'000 mg/l at 20 °C
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation	NA	calculated	In air $T_{1/2}$ = 99.8 hours
3.1.2	Stability in Water			not available
3.3	Transport and Distribution	NA	calculated (Fugacity Level 1 Type)	In Air 22.18 % In Water 77.5 % In Soil 0.31 % In Sediment 0.007 % In susp. Sed. 0.00022 % In Fish 0.000018 %
3.5	Biodegradation	Act. sewage sludge Act. sewage sludge	EEC 79/831 OECD 302B	67% after 28 days (BOD) 98% DOC-elimin. (28 days) > 95 % after 4 days
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	Leuciscus idus L.	DIN 38412 T.15	2150 < LC50 (96hr) < 4640mg/l NOEC = 1000 mg/l
4.2	Acute Toxicity to Aquatic Invertebrates	Daphnia magna	EC 79/831	EC50 (24hr) > 500 mg/l EC50 (48hr) > 500 mg/l
4.3	Toxicity to Aquatic Plants e.g. Algae	Scenedesmus sub-spicatus	DIN 38412 part 9	ErC50 (72hr) > 500 mg/l
4.4	Toxicity to Bacteria	Pseudomonas putida	DIN 38412, T.8	EC50 (17 hr) = 9010 mg/l

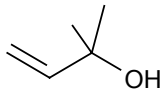
CAS NO: 115-18-4		SPECIES	PROTOCOL	RESULTS
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	not specified	LD50 = 1800 mg/kg
5.1.2	Acute Inhalation Toxicity	Rat	similar to OECD 403	LC50 (4hr) > 21.2 mg/l
5.1.3	Acute Dermal Toxicity	Rabbit	not specified	LD50 > 2000 mg/kg
5.2.1	Skin Irritation	Rabbit	not specified	not irritating
5.2.2	Eye Irritation	Rabbit	not specified	irritating
5.4	Repeated Dose Toxicity	Rat	OECD 407	NOEL = 50 mg/kg LOEL = 200 mg/kg
5.5 A.	Genetic Toxicity in Vitro Bacterial Test (Gene mutation)	Salmonella typhim.	not specified	- with metabolic activation - without metabolic activ.
5.6	Genetic Toxicity in Vivo	Mouse	OECD 474	-
5.8	Toxicity to Reproduction	Rat	OECD 421 (Draft)	NOAEL Parental: 50 mg/kg NOAEL F1 Offspring: 50 mg/kg

SIDS Initial Assessment Report

1 IDENTITY

1.1 Identification of the Substance

CAS Number: 115-18-4
IUPAC Name: 3-Buten-2-ol, 2-methyl-
Molecular Formula: $C_5H_{10}O$
Structural Formula:



Molecular Weight: 86.13
Synonyms: 2-Methyl-3-buten-2-ol
2-Hydroxy-2-methyl-3-butene
Dimethylvinylcarbinol
1,1-Dimethyl-2-propenol
1,1-Dimethylallyl alcohol
Methylbutenol
In this report the synonym Methylbutenol will be used

1.2 Purity/Impurities/Additives

Degree of purity: 98 %

1.3 Physico-Chemical properties

Table 1 Summary of physico-chemical properties

Property	Value
Physical state	liquid
Boiling point	96-98.5°C at 1013 hPa
Vapour pressure	31.3 hPa at 25°C
Water solubility	190'000 mg/l at 20°C
Partition coefficient n-octanol/water (log value)	0.66

2 GENERAL INFORMATION ON EXPOSURE

2.1 Production

Production figures are only available for Switzerland:

1991: 7600 tonnes

1992: 8000 tonnes

1993: 8200 tonnes

1994: 9000 tonnes

2.2 Manufacturing and Distribution

In Switzerland Methylbutenol is produced at a single site by selective hydration of 3-Butyn-2-ol, 2-methyl-, CAS No. 115-19-5 (this chemical is also an OECD HPV chemical, sponsored by Germany), in a closed system without solvent. The crude reaction product is purified in a continuously working distillation chain. The purified Methylbutenol is transferred via pipelines to the storage tanks, from where it is directly pumped off for further transformations. The distillation residue is collected and shipped for incineration.

Methylbutenol is manufactured in a batch-process during 7 days per week, in 3 batches per day. In each batch 2 workers are producing ~ 7.7 tonnes of the chemical.

A small part of the production volume is shipped in 200 l barrels to an other Swiss company, where it is used as a starting material in the synthesis of flavouring agents. The filling operation is performed in a well ventilated area with dedicated technical equipment.

2.3 Uses

Methylbutenol is mainly used as starting material or intermediate in the synthesis of for instance drugs, vitamin A and E, perfumes. A small amount is used as specific attractant in bark beetle traps.

According to Canadian informations Methylbutenol is used in Canada in the manufacture of fragrances and flavouring agentsand for use in a very limited number of household products at an estimated concentration of 1 ppm. For this purpose amounts of < 1 kg/year are imported to Canada.

A product is also listed in a Finnish register containing 100 % methylbutenol. The product is used exclusively as laboratory chemical. No information is available on occupational and environmental exposure. Methylbutenol is not listed in the product registers of Norway, Sweden and Denmark.

Methylbutenol is not produced and imported in the Czech Republic. There was no production reported in the United States in 1994. No use data were found.

2.4 Natural Occurrence

Methylbutenol is a natural constituent of hops. In fresh hops only traces of the chemical were detected. The concentration continuously increased after drying to reach maximum levels (~0.15% equivalent to 150 mg/100 g dry weight) within 2 years of storing at room temperature.

Methylbutenol is also reported to occur in black currents, oranges and grapes.

2.5 Environmental Exposure and Fate

2.5.1 General Discussion

The identified uses of Methylbutenol indicate that the chemical will be released primarily to air. Minor emissions to the water and no emissions to the soil compartment are expected. The chemical will tend to partition preferentially into the water phase due to its high water solubility (Fugacity

Level I calculation: 77.5% in water, 22.2% in air). Volatilisation from the water phase may occur according to the calculated Henry's Law constant.

No experimental data are available concerning the degradation of Methylbutenol in air. Based on the structure of the chemical direct photolysis is not expected. The half-life of the indirect photolysis (reaction with OH radicals) has been calculated to be approx. 100 hours according to the method of Atkinson.

The following results regarding biodegradability are available:

"Ready" test:	67% degradation in 28 days (BOD)
	98% DOC-elimination in 28 days
"Inherent" test:	> 95% in 4 days (DOC)

The results of the available biodegradability tests show that Methylbutenol will be readily biodegraded in the aquatic environment. These biodegradation results, the low partition coefficient log Pow of 0.66 and the high water solubility of 190´000 mg/l indicate that the chemical will not bioaccumulate and adsorption to soils and sediments is unlikely to occur.

Production release

As described in section 2.2 Methylbutenol is produced, purified and transferred in a closed system without any release to the water compartment. A small part of the Swiss production volume is filled in 200 l barrels and shipped to an other company. The vapours which are produced during the filling process are collected by a vacuum system and released without treatment to the atmosphere.

Release from use

In regard to the extremly small amounts of methylbutenol used in household products an eventual release from consumer products is negligible.

Methylbutenol however will be continuously released in small quantities to the air when used as an attractant in bark beetle traps.

2.5.2 Predicted Environmental Concentration

There are no monitoring data available for the aquatic and the air compartment. Therefore the following PEC considerations are based on assumptions.

Each bark beetle trap contains approx. 1.5 g of Methylbutenol and is biologically effective for approx. 6 weeks. This means that 36 mg of active ingredient are released per day from the trap, or 1.5 mg/h. The area where the chemical is active as attractant is described to be 30 m around the trap. Assuming a height diffusion of 5 m the average concentration is calculated to be 0.1 µg/m3 after 1 hour. This value is considered as worst-case-PEC because the diffusion in natural forests will be usually much higher.

In 1992 independent measurements at the production plant have shown that approx. 0.6 kg/h of organic compounds are emitted. 65% of these emissions are contributed to Methylbutenol. The calculation with this value gives an annual release of 3416 kg to the atmosphere. Taking into account the local geographic and climatic conditions, the concentration in the air in the vicinity of the plant is

$cair = (rr \cdot t) / (vw \cdot lh \cdot ws \cdot t) = 3.4 \cdot 10^{-4}$ mg/m^3

rr	=	release rate	=	390 g/h
t	=	time interval	=	1 h
vw	=	valley width	=	800 m
lh	=	layer height	=	200 m
ws	=	mean wind speed	=	2 m/s

2.6 Human Exposure

Based on the available exposure information, the use pattern and the physical-chemical properties, workers which are involved in the production and filling process as well as consumers which are using household products containing Methylbutenol may be exposed.

2.6.1 Occupational Exposure

During the production process there is some exposure when the Methylbutenol-moistened catalyst is recycled and suspended again in a new batch of the starting material. After the reaction the reaction vessel is opened to take samples. The exposure time per working period is estimated to be ~ 15 minutes.

The exposure during the filling process of the 200 l barrels will be very low due to the protective measures at the workplace (removal of the vapors by vacuum systems, protective equipment like gloves and glasses of the involved workers).

2.6.2 Consumer Exposure

Due to the very limited uses of methylbutenol in household products in Canada and the extremly low concentrations no significant consumer exposure is to be expected from these products.

Because hops may contain small quantities of Methylbutenol it can not be excluded that the chemical is also present in beer depending on the amount and the age of the hops used in the brewing process. However no analytical data are available, and it must be assumed that the effects of ethanol for the human health will be much more serious than those of Methylbutenol.

3 HUMAN HEALTH HAZARDS

3.1 Effects on Human Health

3.1.1 Acute Toxicity

Oral:	LD_{50}: 1800 mg/kg body weight (rat)
Inhalation:	LC_{50} (4h) > 21.2 mg/l (rat)
Dermal:	LD_{50} > 2000 mg/kg body weight (rabbit)
Skin irritation:	Not irritating
Eye irritation:	Irritating
Skin sensitisation:	No data

3.1.2 Repeated Dose Toxicity

Oral (gavage): NOEL = 50 mg/kg body weight/day (rat)

LOEL = 200 mg/kg body weight/day (rat)

In a recent Repeated Dose Toxicity study rats were exposed to 50, 200 and 600 mg/kg/day by the oral route. No toxicologically relevant changes were noted in the low dose group. Above this exposure level apparent signs of toxicity were observed.

No Repeated Dose studies by the inhalation route are available.

3.1.3 Mutagenicity

Bacterial test: Ames test using four strains of S. typhimurium (TA98, TA100, TA1535, TA1537)

Negative both with and without metabolic activation.

Non-bacterial test in vivo:

No chromosomal or other damage detected in an oral (gavage) micronucleus assay with mice.

3.1.4 Toxicity for Reproduction

Administration of Methylbutenol at levels up to 200 mg/kg/day throughout a one-generation study (OECD 421, Draft) was without effect on the general reproductive performance of the test animals. The parental and the offspring NOAEL were both considered to be 50 mg/kg body weight/day.

3.1.5 Other Human Health Related Information

Methylbutenol seems to contribute to the sedative action of hops. Administration of 206.5 mg/kg i.p. to rats caused a decline of motility by 50% within two minutes, reaching a maximum response within two hours.

3.2 Initial Assessment for Human Health

Methylbutenol is of low acute toxicity, is not genotoxic, is irritating to the eyes but not to the skin. It has no effect on the general reproductive performance of test animals.

Based on the NOEL of 50 mg/kg/day from the 28 day oral toxicity study in rats, the Estimated Dose of Low Concern (EDLC) can be calculated taking into account an uncertainty factor (UF) of 100 (according to the OECD Provisional Guidance for the Initial Assessment of Health Effects):

EDLC = (NOEL/UF) = 0.5 mg/kg/day.

The estimated environmental human exposure EHE for the general population can be calculated from the estimated air concentration in the vicinity of the production plant ($3.4 \cdot 10^{-4}$ mg/m^3) assuming a daily respiratory volume of 30 m^3 and a weight of 70 kg for an adult person:

EHE = (30 m^3 $\cdot$ $3.4 \cdot 10^{-4}$ mg/m^3) / 70 kg = $1.5 \cdot 10^{-4}$ mg/kg/day

The EDLC / EHE ratio is calculated to be 3300.

This value and the low calculated concentration of Methylbutenol near bark beetle traps (0.1 µg/m^3) indicate that releases of the chemical to the air do not give cause for concern.

The exposure at the workplace during production and distribution is considered to be negligible as long as the ventilation system is properly working and the workers are wearing protective equipment.

4 HAZARDS TO THE ENVIRONMENT

4.1 Aquatic Effects

Results of acute toxicity tests:

Leuciscus idus (golden orfe): 2150 mg/l < LC_{50} (96h) < 4640 mg/l

NOEC = 1000 mg/l

Daphnia magna: EC_{50} (48h) > 500 mg/l

EC_0 (48h) = 500 mg/l

Scenedesmus subspicatus: EC_{50} (72h) > 500 mg/l

All values are based on nominal concentrations. No results from chronic toxicity tests are available. Therefore an assessment factor of 100 (according to the OECD Provisional Guidance for the Initial Assessment of Aquatic Effects) is chosen to calculate a PNEC of 500 mg/l : 100 = 5 mg/l.

4.2 Terrestrial Effects

No exposure to the terrestrial environment is expected.

4.3 Initial Assessment for the Environment

Air: The concentration of Methylbutenol in air is expected to be very low near bark beetle traps and negligible on a regional and global scale. However one should keep in mind that this chemical is a biologically active compound of the natural fauna and very small quantities could therefore influence the behaviour of specific species.

Water: Methylbutenol is of low acute toxicity to algae, Daphnia and fish. A PNEC of 5 mg/l has been derived from the available data. The chemical will degrade quite rapidly in the aquatic environment and shows no tendency for bioaccumulation. There is no release to the water compartment during production and distribution.

5 RECOMMENDATIONS

The chemical is currently of low priority for further work.

Based on the initial assessments for the environment and human health given Methylbutenol does not give cause for concern.

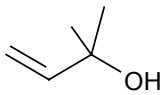
Methylbutenol can be considered to present a low potential for risk to man and the environment

No further studies are required to evaluate potential health and environmental effects.

SIDS DOSSIER

3-BUTEN-2-OL, 2-METHYL-

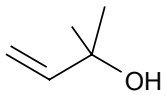
CAS No. 115-18-4



SPONSOR COUNTRY: SWITZERLAND

24 May 1995

1.01 SUBSTANCE INFORMATION

A.	**CAS-number**	115-18-4
B.	**Name** *(IUPAC name)*	3-Buten-2-ol, 2-methyl-
C.	**Name** *(OECD name)*	3-Buten-2-ol, 2-methyl-
E.	**EINECS-Number**	204-068-4
F.	**Molecular Formula**	$C_5H_{10}O$
G.	**Structural Formula**	 Smiles code: C=CC(O)(C)C
J.	**Molecular Weight**	86.13

1.02 OECD INFORMATION

A.	**Sponsor Country:**	Switzerland
B.	**Lead Organisation:**	Federal Office of Environment, Forests and Landscape
	Contact Person:	Dr. G. Karlaganis Federal Office of Environment, Forests and Landscape CH - 3003 Berne Tel. +41 31 322 69 55 Fax +41 31 324 79 78
C.	**Name of Responder:**	Dr. R. Schwob F. Hoffmann - La Roche AG CSED, B. 49/2.027 CH - 4002 Basel

1.1 GENERAL SUBSTANCE INFORMATION

A.	**Type of Substance**	organic
B.	**Physical State** *(at 20°C and 1.013 hPa)*	liquid
C.	**Purity**	98 % (GC)

1.2 SYNONYMS

2-Methyl-3-buten-2-ol
2-Hydroxy-2-methyl-3-butene
3-Hydroxy-3-methylbutene
Methylbutenol
Dimethylvinylcarbinol
Dimethylvinylmethanol
1,1-Dimethyl-2-propenol
α,α-Dimethylallyl alcohol
1,1-Dimethylallyl alcohol
2-Methyl-3-buten-2-yl alcohol

1.3 IMPURITIES

CAS No:	75-85-4
EINECS No:	200-908-9
Name:	2-Butanol, 2-methyl-
Value:	1.8 %
CAS No:	7732-18-5
EINECS No:	231-791-2
Name:	Water
Value:	0.2 %

1.4 ADDITIVES

No additives

1.5 QUANTITY

Switzerland: Production range: 5000 - 10000 t/y

Production	1991: 7600 t
	1992: 8000 t
	1993: 8200 t
	1994: 9000 t

Canada: Import < 1 kg/y (1995)

1.6 LABELLING AND CLASSIFICATION

Labelling

Type:	Provisionally by manufacturers (BASF, Roche)
Symbols:	F, Xn
R-phrases:	R11, R22, R36
S-phrases:	S16, S23
Text of S-phrases:	S16 : Keep away from sources of ignition - No smoking.
	S23: Do not breathe vapour.

Classification

Type:	Provisionally by manufacturers (BASF, Roche)
Category of danger:	Highly flammable
R-phrases:	R11
Type:	Provisionally by manufacturers (BASF, Roche)
Category of danger:	Harmful
R-phrases:	R22, R36

In Switzerland 3-Buten-2-ol, 2-methyl- is classified in poison class 4 (rat, LD_{50} range: 500 - 2000 mg/kg p.o.).

1.7 USE PATTERN

A. General

Type of Use:	*Category:*
(a) type	Non dispersive use
industrial	Chemical industry: chemicals used in synthesis
e.g. intermediates	
use	Intermediates
(b) type	Use resulting in inclusion into or onto matrix
industrial	Public domain
use	Non-agricultural pesticides
(c) type	Wide dispersive use
industrial	Personal and domestic use
use	Household products

Remarks:

(a) Use as starting material or intermediate in the synthesis of for instance drugs, vitamin A and E, perfumes.
(b) Use in 2 products as specific attractant in bark beetle traps.
(c) Use in the manufacture of fragrances and flavouring agents for use in a limited number of household products at an estimated maximum concentration of 1 ppm.

Reference:
(a) Roche, 1990a
(b) Shell, 1991
(c) Lewis, 1996

B. Use in consumer products

Information from other countries:

(a) Denmark: The chemical was not found in three or more products on the Danish market in July 1988.

(b) Finland: In February 1994 there was one product in the Finnish product register containing methylbutenol. It was a 100% 2-methyl-3-buten-2-ol containing product which is used as a laboratory chemical. No specific information was available on occupational or environmental exposure.

(c) Sweden: The chemical was not present in the Swedish Chemical Products Register in 1996.

(d) Norway: The chemical was not registered in the Norwegian Product Register in 1996.

Reference:
(a) Niemelä, 1991
(b) Malm, 1994
(c) Lundbergh, 1996
(d) Jorgensen, 1996

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

In Switzerland no MAK value is set for 3-Buten-2-ol, 2-methyl- in the official MAK list.

1.9 SOURCES OF EXPOSURE

Source: Media of release: Air
Quantities per media: Negligible
Remarks: Switzerland.
Methylbutenol is produced at a single site by selective hydration of 3-Butyn-2-ol, 2-methyl-, CAS No. 115-19-5, in a closed system without solvent. A small part (~ 15 t/y) of the production volume is shipped in 200 l barrels to an other Swiss company, where it is used as a starting material in the synthesis of flavoring agents. The filling operation is performed in a well ventilated area with dedicated technical equipment.
Reference: ROCHE, 1995a

Source: Media of release: Air
Quantities per media: Negligible
Remarks: Germany.
Methylbutenol is the active ingredient in two commercially available bark beetle traps (concentration: ~ 1.5 g per trap). 510 - 1580 kg/y of Methylbutenol have been used for the manufacturing of these traps (1985 - 1991).
Reference: Shell, 1991

1.10 ADDITIONAL REMARKS

A. Options for disposal

Incineration.

B. Other remarks

3-Buten-2-ol, 2-methyl- is a natural pheromone component of the bark beetle species *Ips typographus* (L.) and *Ips (Orthotomicus) erosus*.

Reference: Eidmann *et al*., 1986

2.1 MELTING POINT

Value:	-26°C
Decomposition:	No
Sublimation:	No
Method:	ROCHE internal method
GLP:	No
Reference:	Roche,1990
Value:	-28°C
Decomposition:	No
Sublimation:	No
Method:	BASF internal method
GLP:	No
Reference:	BASF, 1991a

2.2 BOILING POINT

Value:	96 - 98.5°C
Pressure:	at 1013 hPa
Decomposition:	No
Method	DIN 51751
GLP	No
Reference:	BASF, 1991a

2.3 DENSITY

Type:	Relative density
Value:	0.82 g/cm^3
Temperature:	20°C
Method:	DIN 51757
GLP:	No
Reference:	BASF, 1991a

2.4 VAPOUR PRESSURE

Value:	130.2 hPa
Temperature:	50°C
Method:	Dynamic ebulliometric method
GLP:	No
Reference:	Roche, 1990
Value:	31.3 hPa
Temperature:	25°C
Method:	Calculated according to log P(Torr) = A + B/(T(°C)+C) A = 7.6091 B = -1415.4 C = 201.88
Reference:	Roche, 1990
Value:	137 hPa
Temperature:	50°C
Method:	BASF internal method
GLP:	No
Reference:	BASF, 1991a

2.5 PARTITION COEFFICIENT $LOG_{10}P_{OW}$

log Pow:	0.66
Temperature:	25°C
Method:	Measured, OECD 107
GLP:	No
Reference:	BASF, a

2.6 WATER SOLUBILITY

A. Solubility

Value:	190'000 mg/l
Temperature:	20°C
Description:	Of high solubility
Method:	ROCHE internal method
GLP:	No
Reference:	Roche, 1990

B. pH Value, pKa Value

No data available.

2.7 FLASH POINT (liquids)

Value:	11°C
Type of test:	Closed Cup
Method:	DIN 51755
GLP:	No
Reference:	BASF, 1991a

Value:	15°C
Type of test:	Open Cup
Method:	ROCHE internal method (Abel-Pensky)
GLP:	No
Reference:	Roche, 1990

2.8 AUTO FLAMMABILITY (solid/gases)

Not applicable.

2.9 FLAMMABILITY

Not applicable.

The classification "highly flammable" is based on the flash point of the compound (limit value 21°C).

2.10 EXPLOSIVE PROPERTIES

No data available.

2.11 OXIDIZING PROPERTIES

No data available.

2.12 OXIDATION:REDUCTION POTENTIAL

Not applicable.

2.13 ADDITIONAL DATA

Ignition temperature:	380°C
Method:	DIN 51794
Reference:	BASF, 1991a
Flammable limits in air:	1.5% to 9.4%
Reference:	BASF, 1991a

3.1 STABILITY

3.1.1 Photodegradation

Type:	Air
Indirect photolysis:	
Type of sensitizer:	OH radicals
Concentr. of sensitizer:	$5 \cdot 10^5$ radicals/cm^3
Rate constant:	$3.86 \cdot 10^{-12}$ cm^3/molecule · sec
Degradation:	50% in 99.8 hours
Method:	Calculated according to Atkinson
Reference:	Atkinson, 1988

3.1.2 Stability in Water

No studies located.

3-Buten-2-ol, 2-methyl- is not expected to undergo chemical hydrolysis under environmental conditions since it contains no hydrolyzable functional groups.

3.1.3 Stability in Soil

No data

3.2 MONITORING DATA (environmental)

Type of measurement:	Background
Media:	Food
Results:	~ 0.15 %
Remarks:	

In fresh hops only traces of 3-Buten-2-ol, 2-methyl- were detected. The concentration continously increased after drying to reach maximum levels (approx. 0.15 % equivalent to 150 mg/100 g dry weight) within 2 years of storing at room temperature, irrespective of the specific kind of the hop.

Reference: Hänsel *et al.*, 1982

3.3 TRANSPORT AND DISTRIBUTION

3.3.1 Transport

Type:	Volatility
Media:	Water - air
Method:	Calculated according to Lyman *et al.*
Results:	Based on a water solubility of 190'000 mg/l and a vapour pressure of 31.3 hPa, the calculated Henry's Law constant is 1.419 Pa · m^3/mole.
Remarks:	The calculated Henry's Law constant indicates that volatilization from surface waters may be possible.
Reference:	Lyman *et al.*, 1982

3.3.2 Theoretical Distribution (Fugacity Calculation)

Media:	Air-biota-sediment-soil-water
Method:	Fugacity level I

Results:

Distribution	Compartment	Volumes
22.18 %	Air	$1 \cdot 10^{14}$ m^3
77.5 %	Water	$2 \cdot 10^{11}$ m^3
0.31 %	Soil solids	$9 \cdot 10^{9}$ m^3
0.007 %	Sediment solids	$1 \cdot 10^{8}$ m^3
0.00022 %	Suspended sediment	$1 \cdot 10^{6}$ m^3
0.000018 %	Biota (fish)	$2 \cdot 10^{5}$ m^3

Remarks:

Calculation of the theoretical distribution of 3-Buten-2-ol, 2-methyl- in the environment using the FUGMOD model level I, version 1. All the default values were used.

Input data:

Molecular mass g/mol	86.13
Melting point deg C	-26
Vapor pressure Pa	3130
Solubility g/m^3	190000
Log octanol-water p-coefficient	0.66

Reference: FUGMOD, 1992

3.4 IDENTIFICATION OF MAIN MODE OF BIODEGRAD. IN ACTUAL USE

No data.

3.5 BIODEGRADATION

Type:	Aerobic
Inoculum:	Activated sludge, domestic
Concentration:	265 mg/l related to test substance
Medium:	Sewage treatment
Degradation:	67% of the theoretical oxygen demand after 28 days. DOC-elimination: 98% in 28 days
Results:	Readily biodegradable
Method:	Manometric respirometry EEC 79/831 annex V, part C, 5.2 (1984)
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: not specified
Remarks:	Lag-phase: 11 days Degradation phase: 6 days DOC-elimination of the reference substance aniline: 97% after 28 days
Reference:	BASF, 1989b

Type:	Aerobic
Inoculum:	Activated sludge, industrial
Concentration:	265 mg/l related to test substance
Medium:	Sewage treatment
Degradation:	DOC-reduction: > 95% after 4 days
Results:	Inherently biodegradable
Method:	OECD 302B (modified Zahn-Wellens test)
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: 98%
Reference:	BASF, 1989a

3.6 BOD_5, COD OR RATIO BOD_5/COD

BOD_5

Method:	Not reported
Concentration:	649 mg/l related to DOC
Value:	730 mg O_2/l
GLP:	No

COD

Method:	Not reported
Value:	2600 mg O_2/g
GLP:	No

Ratio BOD_5/COD	0.28
Reference:	BASF, 1989b

3.7 BIOACCUMULATION

No data available.

3.8 ADDITIONAL REMARKS

No additional remarks.

4.1 ACUTE / PROLONGED TOXICITY TO FISH

Type of test:	Static
Species:	Golden orfe (Leuciscus idus L., golden variety)
Exposure period:	96 hours
Results:	$2150 < LC_{50}$ (24h) < 4640 mg/l
	$2150 < LC_{50}$ (48h) < 4640 mg/l
	$2150 < LC_{50}$ (72h) < 4640 mg/l
	$2150 < LC_{50}$ (96h) < 4640 mg/l
	NOEC = 1000 mg/l
Analytical monitoring:	No
Method:	DIN 38412 T.15
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: >99%

Remarks:

Maximum concentration tested causing no mortality: 2150 mg/l
Minimum concentration tested causing 100% mortality: 4640 mg/l
Temperature: 21 ± 1°C ; pH 7.4 - 7.8 ; slight aeration
Values based on nominal concentrations

Reference: BASF, 1988a

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

A. Daphnia

Type of test:	Static
Species:	Daphnia magna Straus
Exposure period:	48 hours
Results:	EC_{50} (24h) > 500 mg/l
	EC_0 (24h) = 500 mg/l
	EC_{100} (24h) > 500 mg/l
	EC_{50} (48h) > 500 mg/l
	EC_0 (48h) = 500 mg/l
	EC_{100} (48h) > 500 mg/l
Analytical monitoring:	No
Method:	EC directive 79/831, annex V, C2
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: >99%
Remarks:	Temperature: 19 - 21°C ; pH: 7.9 - 8.1
	Values based on nominal concentrations
Reference:	BASF, 1988b

B. Other aquatic organisms

No studies located.

4.3 TOXICITY TO AQUATIC PLANTS, E.G. ALGAE

Species:	Scenedesmus subspicatus CHODAT
Endpoint:	Growth
Exposure period:	72 hours

Results:

	EC_{20}	EC_{50}	EC_{90}
after 24h:	> 500 mg/l	> 500 mg/l	> 500 mg/l
after 48h:	250 mg/l	> 500 mg/l	> 500 mg/l
after 72h:	300 mg/l	> 500 mg/l	> 500 mg/l

Analytical monitoring: No
Method: DIN 38412 part 9 (Growth rate)
GLP: No
Test substance: 3-Buten-2-ol, 2-methyl-, purity: not specified
Remarks: 23 ± 2°C ; pH 8.7 - 9.1
Values based on nominal concentrations
Reference: BASF, 1989c

4.4 TOXICITY TO BACTERIA

Type: Aquatic
Species: Pseudomonas putida
Exposure period: 17 hours
Results: EC_{10} (17h) = 6260 mg/l
EC_{50} (17h) = 9010 mg/l
EC_{90} (17h) > 10000 mg/l
Analytical monitoring: No
Method: DIN 38412, T.8
GLP: No
Test substance: 3-Buten-2-ol, 2-methyl-, purity: not specified
Reference: BASF, 1991b

Type: Aquatic
Species: Activated sludge, adapted
Exposure period: 30 min
Results: EC_{10} (30 min) > 1000 mg/l
Analytical monitoring: No
Method: ISO 8192
Test for Inhibition of Oxygen Consumption by Activated Sludge
GLP: No
Test substance: 3-Buten-2-ol, 2-methyl-, purity: not specified
Reference: BASF, 1991b

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

No data available

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

No data available

4.7 BIOLOGICAL EFFECTS MONITORING (including Biomagnification)

No information available

4.8 BIOTRANSFORMATION AND KINETICS

No data available

4.9 ADDITIONAL REMARKS

No additional remarks.

5.1 ACUTE TOXICITY

5.1.1 Acute Oral Toxicity

Type:	LD_{50}
Species/strain:	Rat / no data
Value:	1800 mg/kg body weight
Method:	Internal method BASF
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: > 98%
Reference:	BASF, 1991b

Type:	LD_{50}
Species/strain:	Rat / no data
Value:	2280 mg/kg body weight
Method:	Internal method ROCHE
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: > 98%
Reference:	Roche, 1990

5.1.2 Acute Inhalation Toxicity

Type:	LC_{50}
Species/strain:	Rat / no data
Exposure time:	4 hours
Value:	$LC_{50\ (4h)} > 21.2$ mg/l
Method:	Internal method BASF (adaptation of OECD 403)
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: > 98%
Reference:	BASF, b

5.1.3 Acute Dermal Toxicity

Type:	LD_{50}
Species/strain:	Rabbit
Value:	$LD_{50} > 2000$ mg/kg body weight
Method:	Internal method BASF
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: > 98%
Reference:	BASF, b

5.1.4 Acute Toxicity, Other Routes of Administration

Type:	LD_{50}
Species/strain:	Rat / Wistar
Route of administration:	i.p.
Value:	1315 mg/kg body weight
Method:	No data
GLP:	No data
Test substance:	3-Buten-2-ol, 2-methyl-, purity: ≥ 99%

Remarks:	Only males tested LD_{50} is calculated with the Probit method 24 hours *post injectionem* i.p.
Reference:	Wohlfahrt *et al.*, 1993

Type:	LD_{50}
Species/strain:	Mouse / NMRI
Route of administration:	i.p.
Value:	1117 mg/kg body weight
Method:	No data
GLP:	No data
Test substance:	3-Buten-2-ol, 2-methyl-, purity: ≥ 99%
Remarks:	Only males tested LD_{50} is calculated with the Probit method 24 hours *post injectionem* i.p.
Reference:	Wohlfahrt *et al.*, 1993

5.2 CORROSIVENESS / IRRITATION

5.2.1 Skin Irritation / Corrosion

Species/strain:	Rabbit / no data
Results:	Not irritating
Classification:	Not irritating
Method:	Internal method BASF
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: >98%
Reference:	BASF, b

5.2.2 Eye Irritation / Corrosion

Species/strain:	Rabbit
Results:	Irritating
Classification:	Irritating
Method:	Internal method BASF
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: >98%
Reference:	BASF, b

5.3 Skin Sensitisation

No data available

5.4 REPEATED DOSE TOXICITY

Species/strain:	Rat / Wistar
Sex:	Male/Female
Route of administration:	Gavage
Exposure period:	28 days
Frequency of treatment:	Daily, 7 days per week
Post exposure observ. period:	0 and 28 days, respectively
Dose:	50, 200, 600 mg/kg body weight/day 10-14 animals/sex/group
Control group:	Yes, concurrent vehicle

NOEL:	50 mg/kg body weight/day
LOEL:	200 mg/kg body weight/day
Results:	
	No toxicologically relevant changes were seen in the animals treated with 50 mg/kg/day.
	In mid dose females (200 mg/kg/day), minimally increased liver weights and hypertrophy of hepatocytes (1 F) were observed. In mid dose males, the kidney weights were minimally increased and a slight to moderate accumulation of renal hyaline droplets were noted.
	The high dose of 600 mg/kg/day induced sedation, ataxia and uncoordinated gait during the first days of treatment. Salivation was minimally increased after repeated administration. Two animals (1 M, 1 F) died spontaneously. Since no apparent cause of deaths was determined, a treatment-related effect cannot be excluded. No relevant changes in hematological parameters, in ophthalmoscopy and urine analysis were noted. Salient findings were confined to the liver of males and females and to the kidneys of male rats. In males and females, minimally increased liver weights and periacinar hypertrophy of hepatocytes were observed. Transaminases were minimally increased. In male rats minimal increases in kidney weights and tubular accumulation of hyaline droplets were observed. These findings were assigned to the observed $\alpha 2\mu$-Globulin accumulation. It is well known that certain chemicals give rise for such an accumulation and the corresponding relevant changes of the kidney. However this mechanism is highly specific for male rats and not of predictive value for other animal species and for humans. No functional disturbances of the kidneys were noted.
Method:	OECD 407, 1981
GLP:	Yes
Test substance:	3-Buten-2-ol, 2-methyl-, purity: 97.2%
Reference:	Roche, 1994
Species/strain:	Rat / no data
Sex:	No data
Route of administration:	Oral
Exposure period:	5 days
Frequency of treatment:	Daily
Post exposure observ. period:	10 days
Dose:	500, 1000, 2000, 4000 mg/kg body weight (number of animals per dose group not specified)
Control group:	Yes (no details reported)
Results:	LD_{50} = 1410 mg/kg (10 days following 5th administration)
Method:	Internal method ROCHE
GLP:	No

Test substance:	3-Buten-2-ol, 2-methyl-, purity: >98%
Reference:	Roche, 1975

5.5 GENETIC TOXICITY IN VITRO

A. Bacterial Test

Type:	Ames test
System of testing:	Salmonella typhimurium TA98, TA100, TA1535, TA1537
Concentration:	Not specified
Metabolic activation:	With and Without
Results:	Negative
Cytotoxicity conc:	With metabolic activation: not reported Without metabolic activation: not reported
Precipitation conc:	Not reported
Genotoxic effects:	+ ? - With metabolic activation [ ] [ ] [x] Without metabolic activation [ ] [ ] [x]
Method:	Internal method BASF. Standard plate test and preincubation test
GLP:	No
Test substance:	3-Buten-2-ol, 2-methyl-, purity: >98%
Reference:	BASF, c

B. Non-Bacterial in Vitro Test

No data available

5.6 GENETIC TOXICITY IN VIVO

Type:	Micronucleus assay
Species/strain:	Mice / NMRI
Sex:	Male/Female
Route of administration:	Gavage
Exposure period:	Single dose; volume 10 ml/kg body weight
Doses:	500, 1000, 1500 mg/kg body weight Solvent control: 10 ml/kg body weight aqua dest. Positive controls: 20 mg/kg body weight cyclophosphamide 0.15 mg/kg body weight vincristine
Results:	Negative
Genotoxic effects:	+ ? - [ ] [ ] [x]
Method:	In accordance with OECD 474 and Directive 84/449/EEC, B.12
GLP:	Yes
Test substance:	3-Buten-2-ol, 2-methyl-, purity: 97.9%
Remarks:	The administration of the test substance in doses of 1500, 1000 and 500 mg/kg body weight led to evident signs of toxicity like irregular respiration, piloerection and in few

cases apathy.None of these signs or symptoms could be observed on the 1st day after treatment in the 500 mg/kg group, whereas in the two other groups few cases of piloerection were still evident on the 2nd day after treatment.
The single administration of the three doses did not lead to any increase in the number of polychromatic erythrocytes containing either small or large micronuclei. No inhibition of erythropoiesis determined from the ratio of polychromatic to normochromatic erythrocytes was detected.

Reference: BASF, 1992

5.7 CARCINOGENICITY

No data available

5.8 TOXICITY TO REPRODUCTION

Type:	One generation study
Species/strain:	Rats / Fü-Albino (RORO)
Sex:	Male/Female
Route of administration:	Gavage
Exposure period:	~ 22 days
Frequency of treatment:	Daily
Premating exposure period:	2 weeks for male rats (9 weeks old) 2 weeks for female rats (9 weeks old)
Duration of the test:	~ 54 days
Doses:	12.5, 50 and 200 mg/kg/day 10 females and 10 males per group
Control group:	Yes, concurrent vehicle
NOAEL Parental:	50 mg/kg/day
NOAEL F1 Offspring:	50 mg/kg/day
Results:	

P-Generation
The male body weights tended to be reduced at 200 mg/kg/day, but were unaffected at 12.5 or 50 mg/kg/day, when compared to the concurrent controls. The female body weights were comparable among all experimental groups during premating, gestation and lactation.

There were no compound-related abnormal clinical signs in any sex, apart from a slightly increased incidence of 'pasty faeces' at 200 mg/kg/day in males and females, during and after the mating period.

During the premating period the mean food consumption did not differ considerably in both sexes between treated groups and controls. During the lactation period no biologically relevant effects on the female food consumption was observed up to 50 mg/kg/day, whereas there was a slight compound-related decrease at 200 mg/kg/day (mean and median values).

There were no parental necropsy observations considered to be compound-related.

The mating and fertility indices of males and females were comparable in all experimental groups. The mean mating time (i.e. the number of mating days until day 0 of gestation) was slightly prolonged at 50 mg/kg/day.

There were no biologically relevant differences in the reproduction parameters measured between treated groups and controls (mean numbers of: corpora lutea, implantations, pups per litter; resorption rates, mean gestation lengths, mean pup weights, pup sex ratios).

The testes weights were not adversely affected in any of the dose groups.

F1-Generation
At 200 mg/kg/day the pup viability index was reduced by nearly 23% (i.e. the number of pups dying during lactation was increased and the number of pups surviving day 5 of lactation was decreased).

There were no compound-related adverse clinical findings in the pups in any of the dose groups.

Pup body weight at birth and weight development until sacrifice was comparable between treated groups and concurrent controls.

No abnormal findings were observed at the macroscopic external examination of the pups in any experimental group. The visceral examination of the pups of the control (stillborn and died) and the high dose group (all pups) did not indicate any compound-related adverse effects on the morphological development of the offspring.

Method: OECD 421 (Draft), 1994
GLP: Yes
Test substance: 3-Buten-2-ol, 2-methyl-, purity: 97.2%
Reference: Roche, 1995b

5.9 DEVELOPMENTAL TOXICITY / TERATOGENICITY

No data available

5.10 OTHER RELEVANT INFORMATION

A. Specific toxicities

Type: Behaviour
Remarks:

The central nervous system depressant activity of 2-Methyl-3-buten-2-ol was studied by motility tests in order to clarify if it contributes to the sedative action of hops. The substance administered to wistar-rats caused a decline

	of motility by 50% when given i.p. at a dose of 206.5 mg/kg. The onset of activity occurs within two minutes reaching a maximum response within two hours.
Reference:	Wohlfahrt *et al.*, 1993

Atkinson, R. (1988). Estimation of Gas-Phase Hydroxyl Radical Rate Constants for Organic Chemicals. *Environ. Toxicol. Chem. 7*, 435-442.

BASF (a). Analytical laboratory. Unpublished report J. Nr. 124836.1.

BASF (b). Unpublished report # XXII/49.

BASF (c). Unpublished report # 89/43.

BASF (1988a). Unpublished report # 10F0070/885156. December 1988.

BASF (1988b). Unpublished report # 1/0104/2/88. February 1988.

BASF (1989a). Unpublished report J. Nr. 302806. March 1989.

BASF (1989b). Unpublished report. January 1989.

BASF (1989c). Unpublished report # 01/88/1007. October 1989.

BASF (1991a). Material Safety Data Sheet.

BASF (1991b). AIDA Grunddatensatz. March 1991.

BASF (1992). Unpublished report. Project 26M0809/894494. June 1992.

Eidmann H. H., Weslien J., Harding S., Baeckström P., Norin T. and Vrkoc J. (1986). A Compound Replacing a Natural Pheromone Component of the Spruce Bark Beetle. *Naturwissenschaften 73*, 629-630.

FUGMOD (1992). Fugacity level I, II and III Programs for OECD Workshop. Version 1.

Hänsel R., Wohlfart R. and Schmidt H. (1982). Contents of 2-Methyl-3-butene-2-ol in Hops and Hop Preparations. *Planta medica 45*, 224-228.

Jorgensen G.(1996). Letter from Norwegian Pollution Control Authority SFT, Oslo. 22th August 1996.

Lewis M. (1996). Fax from Environment Canada, Québec. 26th June 1996.

Lundbergh I. (1996). Letter from National Chemicals Inspectorate KEMI, Solna. 30th August 1996.

Lyman W. J., Reehl W. F. and Rosenblatt D. H. (1982). *Handbook of Chemical Property Estimation Methods*. McGraw-Hill Book Company.

Malm J. (1994). Letter from the National Board of Waters and the Environment, Chemicals Control Unit, Helsinki. 8th February 1994.

Niemelä J. (1991). Letter from the National Agency of Environmental Protection, Copenhagen. 18th April 1991.

Roche (1975). Internal communication. November 1975.

Roche (1990). F. Hoffmann-La Roche Ltd, Basel. Unpublished report.

Roche (1990a). R+D Memorandum No. B-102349. 23rd February 1990.

Roche (1994). Four-Week Oral (Gavage) Toxicity Study in Rats with Methylbutenol. Unpublished research report No. B-161'217. F. Hoffmann-LaRoche, Basel. 6th December 1994.

Roche (1995a). Exposure data.

Roche (1995b). Reproduction/Developmental Toxicity Screening Test in the Rat with Oral Administration of Methylbutenol. Unpublished research report No. B-161'862. F. Hoffmann-LaRoche, Basel. 10th January 1995.

Shell (1991). Letter from Shell Agrar GmbH, Ingelheim. 19th December 1991.

Wohlfahrt R., Hänsel R. and Schmidt H. (1993). Pharmacology of 2-Methyl-3-buten-2-ol. *Planta medica 48*, 120-123.